Variance minimization variational Monte Carlo method

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We present a variational Monte Carlo (VMC) method that works equally well for the ground and the excited states of a quantum system. The method is based on the minimization of the variance of energy, as opposed to the energy itself in standard methods. As a test, it is applied to the investigation of the universal spectrum at the van der Waals length scale for two identical Bose atoms in a symmetric harmonic trap, with results compared to the basically exact results obtained from a multiscale quantum-defect theory.

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I. INTRODUCTION

Monte Carlo methods have played an important role in our understanding of a variety of quantum systems, especially few- and many-body quantum systems with strong interactions that are difficult to treat otherwise (see, e.g., Refs. [1, 2, 3, 4, 5, 6]). It is also well-known, however, that most quantum Monte Carlo methods [2, 3] are formulated in such a way that they are strictly applicable only to the ground state of a quantum system, a restriction that has severely limited their applicability. Consider, for example, the gaseous Bose-Einstein condensates (BEC) of alkali-metal atoms (see, e.g., [7]). Any theory that intends to treat the real atomic interaction has to deal with the fact that the gaseous BEC branch of states are in fact highly excited states of a many-atom system. There are many branches of states of lower energies, including the first branch of liquid states as suggested and studied recently by one of us [8].

In this paper we present a variational Monte Carlo (VMC) method that works the same way for either the ground or the excited states of a quantum system. It is based on the minimization of the variance of energy, and is the method underlying a recent investigation of the universal equation of state at the van der Waals length scale [8, 9] for few atoms in a trap [10]. The details of the method were skipped in the earlier article [10], both because the focus there was on a single gaseous BEC state, which was not the best example illustrating the method, and because there were no other independent results to directly compared with, except in the shape-independent limit [10].

We present here, in Sec. II, the details of the variational Monte Carlo method based on the minimization of the variance of energy and shows that it applies equally well to the ground and the excited states of a quantum system. In Sec. III, we present a better illustration of the method through the universal spectrum at the van der Waals length scale for two identical Bose atoms in a symmetric harmonic trap. It is an example where results for multiple energy levels can be obtained independently using other methods [11, 12, 13, 14], including, in particular, a multiscale quantum-defect theory (QDT) [15, 16]. Conclusions are given in Sec. IV. We point out that in the process of writing this article, we have discovered that an equivalent approach has been developed earlier by Umrigar *et al.* [17]. The derivation of our method, and the applications presented here and earlier [10], are however different.

II. VARIANCE MINIMIZATION VARIATIONAL MONTE CARLO METHOD

Consider the time-independent Schrödinger equation

$$\widehat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle , \qquad (1)$$

where the energy eigenstates $\left|\Psi_n\right\rangle$ form a complete, orthonormal basis.

Existing quantum Monte Carlo methods are mostly based on the fact that for an arbitrary trial wave function satisfying proper boundary conditions, we have

$$E_T[\Psi_T] \equiv \frac{\left\langle \Psi_T \left|\widehat{H}\right| \Psi_T \right\rangle}{\left\langle \Psi_T | \Psi_T \right\rangle} \geq E_0 , \qquad (2)$$

which means that the ground state wave function is the one that minimizes the energy functional $E_T[\Psi_T]$. The proof can be found in standard quantum mechanics textbooks (see, e.g., [18]).

The variance minimization variational Monte Carlo method (VMVMC), as proposed here, is based on the functional

$$\eta[\Psi_T] \equiv \frac{\left\langle \Psi_T \left|\widehat{H}^2\right| \Psi_T \right\rangle}{\left\langle \Psi_T | \Psi_T \right\rangle} - \left[\frac{\left\langle \Psi_T \left|\widehat{H}\right| \Psi_T \right\rangle}{\left\langle \Psi_T | \Psi_T \right\rangle}\right]^2 \geq 0 . \quad (3)$$

The proof of Eq. (3) and its physical meaning can be best understood by expanding the trial wave function using the complete basis defined by Eq. (1) to write $\eta[\Psi_T]$ as

$$\eta[\Psi_T] = \frac{\sum_m |\langle\Psi_m|\Psi_T\rangle|^2 \, (E_m - E_T)^2}{\sum_m |\langle\Psi_m|\Psi_T\rangle|^2} . \qquad (4)$$

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From Eq. (4), it is clear that zero is the minimum of the functional $\eta[\Psi_T]$, and this minimum is reached when and only when $E_T = E_n$ and $\langle \Psi_m | \Psi_T \rangle = 0$ for $m \neq n$, namely, only when $|\Psi_T\rangle$ is an eigenstate of energy as defined by Eq. (1). This statement is equally applicable to the ground and the excited states of a quantum system.

The implementation of VMVMC, based on the minimization of the variance of energy $\eta[\Psi_T]$, is straightforward. It does not require much more than the standard VMC, as we illustrate here using the example of identical particles.

Consider N identical particles in an external potential and interacting via pairwise interactions. It is described by a Hamiltonian:

$$\widehat{H} = \sum_{i=1}^{N} \hat{h}_i + \sum_{i<j=1}^{N} v(r_{ij}) , \qquad (5)$$

with

$$\hat{h}_i = -\frac{\hbar^2}{2m}\nabla_i^2 + V_{ext}(\mathbf{r}_i) . \qquad (6)$$

Here $V_{ext}(\mathbf{r})$ is the external "trapping" potential, and $v(r)$ is the interaction between particles.

For the evaluation of the energy functional, we have

$$\langle \Psi_T | \widehat{H} | \Psi_T \rangle = \langle \Psi_T | N\hat{h}_1 + \frac{1}{2}N(N-1)v_{12} | \Psi_T \rangle$$
$$= \int d\tau \Psi_T^* \Psi_T \frac{1}{\Psi_T}\{N\hat{h}_1 + \frac{1}{2}N(N-1)v(r_{12})\}\Psi_T$$
$$= \int d\tau \Psi_T^* \Psi_T E_{Loc}(\tau) , \qquad (7)$$

where τ represents an N particle configuration specified by their $3N$ coordinates. E_{Loc} is the so-called local energy, and is given by

$$E_{Loc} = N\left(-\frac{\hbar^2}{2m}\right)\frac{1}{\Psi_T}\nabla_1^2\Psi_T + NV_{ext}(\mathbf{r}_1) + \frac{1}{2}N(N-1)v(r_{12}) \qquad (8)$$

The average energy is therefore

$$E_T = \frac{\int d\tau \Psi_T^* \Psi_T E_{Loc}(\tau)}{\int d\tau \Psi_T^* \Psi_T} . \qquad (9)$$

This is the standard integral in VMC, and can be evaluated using standard Monte Carlo methods such the Metropolis method (see, e.g., [19]).

In order to calculate the variance of energy, one must also determine the average of $\widehat{H}^2$. This can be done by first noting that, similar to Eq. (7), we have

$$\langle \Psi_m | \widehat{H} | \Psi_T \rangle = \int d\tau \Psi_m^* \Psi_T E_{Loc}(\tau) , \qquad (10)$$

where $|\Psi_m\rangle$ is an eigenstate of energy as defined by Eq. (1). We have therefore

$$\langle \Psi_T | \widehat{H}^2 | \Psi_T \rangle = \sum_m \langle \Psi_T | \widehat{H} | \Psi_m \rangle \langle \Psi_m | \widehat{H} | \Psi_T \rangle$$

$$= \sum_m \langle \Psi_m | \widehat{H} | \Psi_T \rangle^* \langle \Psi_m | \widehat{H} | \Psi_T \rangle$$
$$= \sum_m \int d\tau d\tau' [\Psi_m(\tau')\Psi_T^*(\tau')E_{Loc}^*(\tau')$$
$$\times \Psi_m^*(\tau)\Psi_T(\tau)E_{Loc}(\tau)] . \qquad (11)$$

Using the completeness relation

$$\sum_m \Psi_m(\tau')\Psi_m^*(\tau) = \delta(\tau' - \tau) , \qquad (12)$$

we obtain

$$\langle \Psi_T | \widehat{H}^2 | \Psi_T \rangle = \int d\tau \Psi_T^*(\tau)\Psi_T(\tau)|E_{Loc}(\tau)|^2 , \qquad (13)$$

and therefore

$$\frac{\langle \Psi_T | \widehat{H}^2 | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} = \frac{\int d\tau \Psi_T^*(\tau)\Psi_T(\tau)|E_{Loc}(\tau)|^2}{\int d\tau \Psi_T^*(\tau)\Psi_T(\tau)} . \qquad (14)$$

The computation of the variance of energy, Eq. (3), has thus been reduced to two integrals, Eqs. (7) and (14), both of which involving the same local energy, E_{Loc}, that one encounters in standard VMC. It is clear that the formulation and the equations in this section are applicable to both bosons and fermions.

One can easily show that our method is equivalent to that of Umrigar _et al._ [17]. However, we believe that our derivation provides a more rigorous foundation and shows more explicitly why it works for both the ground and the excited states.

III. SAMPLE RESULTS FOR IDENTICAL BOSE ATOMS IN A SYMMETRIC HARMONIC TRAP

The VMVMC, as outlined in Sec. II, was first applied in Ref. [10] to study the universal equation of state at the van der Waals length scale [8, 9] for few identical Bose atoms (N = 3-5) in a trap. To better illustrate and to further test the method, we investigate here the universal spectrum at the van der Waals length scale for two identical Bose atoms in a symmetric harmonic trap. It is a problem for which accurate results can be obtained independently using a variety of methods [11, 12, 13, 14], including a multiscale QDT [15, 16].

Two identical Bose atoms in a symmetric harmonic trap are described by the Hamiltonian, Eqs. (5)-(6), with $N = 2$, and

$$V_{ext}(\mathbf{r}_i) = \frac{1}{2}m\omega^2 r_i^2 , \qquad (15)$$

where m is the mass of an atom, and ω is the trap frequency.

For the trap states of interest here, we take the trial wave function to be of the form of

$$\Psi_T = [\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) + \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)] F(r_{12}) , \qquad (16)$$

where ϕ_1 and ϕ_2 are independent-particle orbitals, and F is the atom-atom correlation function that is discussed in more detail in Ref. [10]. Specifically, we use

$$F(r) = \begin{cases} Au_\lambda(r)/r & , \ r < d \\ (r/d)^\gamma & , \ r \geq d \end{cases} , \qquad (17)$$

where $u(r)$ satisfies the Schrödinger equation:

$$\left[-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + v(r) - \lambda \right] u_\lambda(r) = 0 , \qquad (18)$$

for $r < d$. γ is the parameter characterizing the long-range correlation between atoms in a trap, with $\gamma = 0$ (meaning $F = 1$ for $r > d$) corresponding to no long-range correlation. Both d and γ are taken to be variational parameters, in addition to the variational parameters associated with the descriptions of ϕ_1 and ϕ_2. The parameters A and λ are not independent. They are determined by matching F and its derivative at d. Our choice of F differs from traditional choices (see, e.g. Ref. [6]) not only in its treatment of the short-range correlation, but especially in its allowance for the long-range correlation characterized by parameter γ. This was first suggested by a multiscale QDT treatment of two atoms in a symmetric harmonic trap [15, 16], and was later found to be the key for treating N trapped atoms in cases of strong coupling, namely when the s wave scattering length a_0 becomes comparable to or greater than the trap length scale $a_{ho} = (\hbar/m\omega)^{1/2}$ [10].

For atoms in their ground state, the atom-atom interaction is of the van der Waals type of $-C_n/r^n$ with $n = 6$ at large interatomic separations, i.e.,

$$v(r) \overset{r\to\infty}{\longrightarrow} -C_6/r^6 . \qquad (19)$$

This interaction has an associated length scale of $\beta_6 = (mC_6/\hbar^2)^{1/4}$, and a corresponding energy scale of $s_E = (\hbar^2/m)(1/\beta_6)^2$ [20]. Over a wide range of energies that is hundreds of s_E around the threshold [21, 22], the details of atomic interactions of shorter range than β_6 are not important, and can be characterized by a single parameter that can be the s wave scattering length a_0, the short range K matrix K^c, or some other related parameters [21, 23, 24]. In this range of energies, the spectrum of two atoms in a trap follows a universal property that can be characterized by [10, 15, 16]

$$\frac{E_i/N}{\hbar\omega} = \Omega_i(a_0/a_{ho}, \beta_6/a_{ho}) , \qquad (20)$$

and is called the universal spectrum at length scale β_6. Here Ω_i are universal functions that are uniquely determined by the number of particles, the exponent of the van der Waals interaction ($n = 6$), and the exponent of the trapping potential (2 for the harmonic trap). The strengths of interactions, characterized by C_6 and ω, play a role only through scaling parameters such as β_6 and a_{ho}.
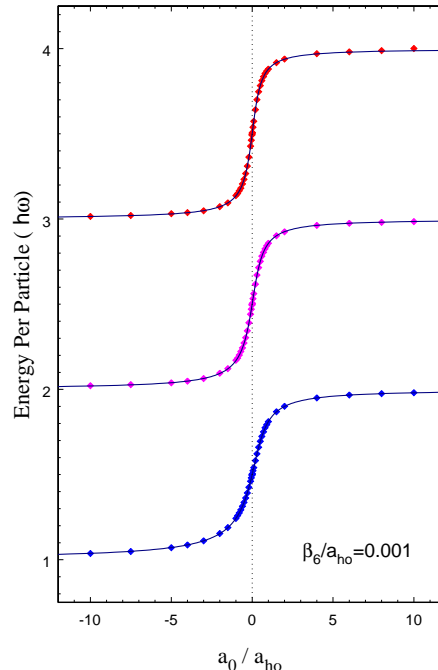

FIG. 1: The universal spectrum at length scale β_6 for two Bose atoms in a symmetric harmonic trap as a function of a_0/a_{ho} for $\beta_6/a_{ho} = 0.001$. Solid line: results from a multiscale QDT [16]. Symbols: results of VMVMC.

As in Ref. [10], the universal spectrum at length scale β_6, namely the Ω_i's in Eq. (20), can be computed by using a correlation function, Eq. (17), with $u_\lambda(r)$ as given by the angular-momentum-insensitive quantum-defect theory (AQDT) [21],

$$u_{\lambda_s}(r_s) = B[f^{c(6)}_{\lambda_s l=0}(r_s) - K^c g^{c(6)}_{\lambda_s l=0}(r_s)] . \qquad (21)$$

Here B is a normalization constant. $f^{c(6)}_{\lambda_s l}$ and $g^{c(6)}_{\lambda_s l}$ are universal AQDT reference functions for $-C_6/r^6$ type of potentials [9, 20]. They depend on r only through a scaled radius $r_s = r/\beta_6$, and on energy only through a scaled energy $\lambda_s = \lambda/s_E$. K^c is the short-range K matrix [21] that is related to the s wave scattering length a_0 by [24, 25]

$$a_0/\beta_n = \left[b^{2b}\frac{\Gamma(1-b)}{\Gamma(1+b)} \right] \frac{K^c + \tan(\pi b/2)}{K^c - \tan(\pi b/2)} , \qquad (22)$$

where $b = 1/(n-2)$, with $n = 6$.

Figure 1 shows a portion of the universal spectrum at length scale β_6 for two Bose atoms in a symmetric harmonic trap. Specifically, it gives the energies of the first three s wave trap states as a function of a_0/a_{ho}. The corresponding ϕ_is used in Eq. (16) are independent-particle orbitals based on standard solutions for a single particle in a symmetric harmonic potential (see, e.g., [26]). For
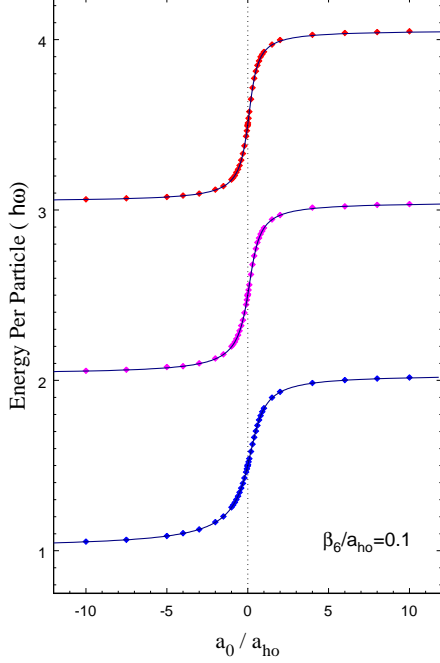
FIG. 2: The same as Fig. 1 except for $\beta_6/a_{ho} = 0.1$.

FIG. 3: A comparison of the spectra for two different values of β_6/a_{ho}, illustrating the shape-dependent correction that becomes more important for greater values of β_6/a_{ho} and for more highly excited states.

the lowest s wave trap state, they are taken to be

$$\phi_i(\mathbf{r}) = exp(-\alpha_i x^2) \ , \ i = 1, 2. \qquad (23)$$

They are taken to be

$$\begin{aligned} \phi_1(\mathbf{r}) &= exp(-\alpha_1 x^2) \ , \\ \phi_2(\mathbf{r}) &= \left(\frac{3}{2} - x^2\right) exp(-\alpha_2 x^2) \ , \end{aligned} \qquad (24)$$

for the first excited s wave trap state, and

$$\phi_i(\mathbf{r}) = \left(\frac{3}{2} - x^2\right) exp(-\alpha_i x^2) \ , \ i = 1, 2, \qquad (25)$$

for the second excited s wave trap state. Here x is a scaled radius defined by $x = r/a_{ho}$. The variational parameters are d, γ, α_1, and α_2 in all three cases. The variance of energy is calculated according to Sec. II, and the minimization is carried out using a type of genetic algorithm.

Both Figs. 1 and 2 show that the results of VMVMC are in excellent agreements with those of a multiscale QDT [15, 16], which gives basically exact results for two atoms in a symmetric harmonic trap. (The scaled energy per particle, $E_i/(2\hbar\omega)$, used here is related to the scaled center-of-mass energy, $e = \epsilon/\hbar\omega$, used in Ref. [16], by $E_i/(2\hbar\omega) = (e + 3/2)/2$.) The agreements are all within the variances of energy, which are smaller for weaker coupling (smaller a_0/a_{ho}) and greater for stronger coupling,
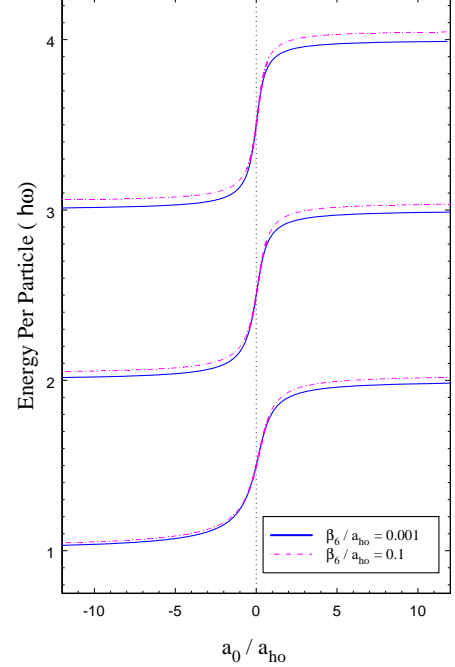
but are in any case less than 1.8×10^{-3} for all parameters considered. The results shown in Figure 1, which are for a small $\beta_6/a_{ho} = 0.001$, illustrate the shape-independent limit of $\beta_6/a_{ho} \rightarrow 0$ for states with $E_i/2 \sim \hbar\omega \ll s_E$ [10, 16]. They agree, in this limit, with the results obtained using a delta-function pseudopotential [11]. For greater β_6/a_{ho}, the effects of the van der Waals interaction become gradually more important, especially for strong coupling ($a_0/a_{ho} \sim 1$ or greater) and for more highly excited states [12, 16]. This is illustrated in Figure 3, which compares the results for $\beta_6/a_{ho} = 0.1$ with those for $\beta_6/a_{ho} = 0.001$. We note that even the lowest trap state is itself a highly excited diatomic state. There are other "molecular" states that are lower in energy [15, 16]. This fact does not, however, lead to any difficulties because VMVMC works the same for the ground and the excited states. It is for the same reason that we were able to investigate the gaseous BEC state for few atoms in a trap [10], which is again a highly excited state. More detailed discussions of the universal spectrum at length scale β_6 for two atoms in a symmetric harmonic trap, including the molecular states and the spectra for nonzero partial waves, can be found elsewhere [16].

IV.   CONCLUSIONS

We have presented a variational Monte Carlo method, VMVMC, that works the same for the excited states as it does for the ground state. The method is tested here through the universal spectrum at length scale β_6 for two identical Bose atoms in a symmetry harmonic trap, for which the results from VMVMC are found to be in excel-lent agreements with the basically exact results derived independently from a multiscale QDT [15, 16].

[1] M. H. Kalos, D. Levesque, and L. Verlet, Phys. Rev. A **9**, 2178 (1974).

[2] D. M. Ceperley, Rev. Mod. Phys. **67**, 279 (1995).

[3] W. M. C. Foulkes, L. Mitas, R. J. Needs, and G. Rajagopal, Rev. Mod. Phys. **73**, 33 (2001).

[4] S. Giorgini, J. Boronat, and J. Casulleras, Phys. Rev. A **60**, 5129 (1999).

[5] D. Blume and C. H. Greene, Phys. Rev. A **63**, 063601 (2001).

[6] J. L. DuBois and H. R. Glyde, Phys. Rev. A **63**, 023602 (2001).

[7] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).

[8] B. Gao, Phys. Rev. Lett. **95**, 240403 (2005).

[9] B. Gao, J. Phys. B **37**, L227 (2004).

[10] I. Khan and B. Gao, Phys. Rev. A **73**, 063619 (2006).

[11] T. Busch, B.-G. Englert, K. Rzazewski, and M. Wilkens, Found. Phys. **28**, 549 (1998).

[12] E. Tiesinga, C. J. Williams, F. H. Mies, and P. S. Julienne, Phys. Rev. A **61**, 063416 (2000).

[13] D. Blume and C. H. Greene, Phys. Rev. A **65**, 043613 (2002).

[14] E. L. Bolda, E. Tiesinga, and P. S. Julienne, Phys. Rev. A **66**, 013403 (2002).

[15] Y. Chen and B. Gao, Bull. Am. Phys. Soc. **50**, No. 3, 80 (2005).

[16] Y. Chen and B. Gao, cond-mat/0701384.

[17] C. J. Umrigar, K. G. Wilson, and J. W. Wilkins, Phys. Rev. Lett. **60**, 1719 (1988).

[18] J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, New York, 1994).

[19] J. M. Thijssen, *Computational Physics* (Cambridge University Press, Cambridge, 1999).

[20] B. Gao, Phys. Rev. A **58**, 1728 (1998).

[21] B. Gao, Phys. Rev. A **64**, 010701(R) (2001).

[22] B. Gao, E. Tiesinga, C. J. Williams, and P. S. Julienne, Phys. Rev. A **72**, 042719 (2005).

[23] B. Gao, Phys. Rev. A **58**, 4222 (1998).

[24] B. Gao, Euro. Phys. J. D **31**, 283 (2004).

[25] B. Gao, J. Phys. B **36**, 2111 (2003).

[26] N. Zettili, *Quantum Mechanics* (John Wiley and Sons, New York, 2001).